

Breit–Pauli energy levels and transition rates for the carbonlike sequence

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Abstract: Breit–Pauli results for energy levels, lifetimes, and some transition data are reported for all levels up to $2s^22p3d\ ^1P_J^o$ of the C-like spectrum for $7 \leq Z \leq 15$. For all but the lowest members of the sequence, these include all the states of the $2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p3s$, $2s^22p3p$, and $2s^22p3d$ configurations. For carbon, only the states for the $2s^22p^2$, $2s2p^3$, and $2s^22p3s$ configurations are included. A simultaneous optimization scheme was applied so that a radial basis could be determined for a set of terms that mix in the Breit–Pauli approximation. All results have been posted at a Web site. In this paper, lifetimes are reported and, in addition, results for N II, O III, and Si IX are critically evaluated. Energy levels are compared with experiment and adjusted transition rates, along with uncertainty estimates are presented. Selected results are compared with other theory and experiment.

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Résumé : Nous avons obtenu les valeurs Breit–Pauli pour les niveaux d'énergie, les demi-vies et les données de transition pour tous les niveaux jusqu'au $2s^22p3d\ ^1P_J^o$ des ions de type carbone avec $7 \leq Z \leq 15$. Pour tous les membres de la séquence, sauf les plus bas, ceux-ci incluent tous les états des configurations $2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p3s$, $2s^22p3p$ et $2s^22p3d$. Pour le carbone, seuls les états des configurations $2s^22p^2$, $2s2p^3$ et $2s^22p3s$ sont inclus. Nous avons utilisé une méthode d'optimisation simultanée afin de déterminer une base radiale pour un ensemble de termes qui se mélangent dans l'approximation de Breit–Pauli. Tous les résultats apparaissent sur une page web. Ici, nous donnons les demi-vies et évaluons méticuleusement les résultats pour N II, O III et Si IX. Les niveaux d'énergie sont comparés aux valeurs expérimentales, ainsi que les taux de transition, incluant des estimés des incertitudes. Quelques résultats choisis sont comparés avec d'autres théories et avec les résultats expérimentaux.

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1. Introduction

Carbon, nitrogen, and oxygen are abundant elements in the Universe, often observed in astrophysical objects, including the Earth's atmosphere. Emission lines of carbonlike ions are useful in the diagnosis of the solar, astrophysical, and fusion plasmas whose interpretation requires accurate atomic data. Decay from the $2s^22p3d\ ^3P_2^o$ level in the O III level is particularly important in the study of the Bowen fluorescence mechanism [1].

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Table 1. Optimization strategies for groups of terms. Eigenfunctions for a specific term are designated by the dominant configuration. All weights are unity unless designated otherwise in parentheses following the term.

Groups	Additional terms or eigenfunctions	
Even		
$2s^22p^2$	3P , 1D , 1S	$2s^22p3p$ 3P , 1P , 1S (all 0.5)
$2p^4$	3P , 1D , 1S	
$2s2p3p$	3P , 1D , 1S , 1P , 3D , 3S	$2s^22p^2$ 3P , 1D , 1S (all 0.5)
Odd		
$2s2p^3$	$^5S^o$, $^3D^o$, $^3P^o$, $^1D^o$, $^3S^o$, $^1P^o$	$2s^22p3s$ $^1P^o$, $^3P^o$ (all 0.5)
$2s^22p3s$	$^1P^o$, $^3P^o$	$2s2p^3$ $^3D^o$, $^3P^o$, $^1D^o$, $^1P^o$ (all 0.5)
$2s^22p3d$	$^3F^o$, $^1D^o$, $^3D^o$, $^3P^o$, $^1F^o$, $^1P^o$	

Currently, it is customary to study a single transition when it presents a particular challenge such as cancellation in the $3s - 4p$ transition of Mg^+ [2] or in the case of intercombination lines as in $2s^22p^2$ $^3P_{1,2} - 2s2p^3$ $^5S_2^o$ of N II where term mixing is crucial [3]. But the last decade has also seen “spectrum” calculations, motivated largely by the extensive data needs of the Opacity project, where all the levels of a portion of the spectrum are computed along with transition rates or oscillator strength for transitions between the levels. An example is the calculation for neutral carbon, which includes all levels up to $2s^22p3d$ [4]. The importance of correlation is well known and orbitals up to $5g$ were included in the calculation. But relativistic effects were expected to be smaller; included were the mass correction, the Darwin terms, and the fine-structure splitting, approximated by the operator

$$\frac{1}{2}\alpha^2 \sum_1^N \zeta_l \frac{1}{r^3} (\mathbf{l}_l \cdot \mathbf{s}_l) \quad (1)$$

where $\zeta_l = 0.55Z\delta_{l,1}$. This approximation may be adequate for energies, but it may happen that the two-body Breit–Pauli operators that have been omitted mix a term with a much larger dipole matrix element than that of the main transition, in which case the transition rates will have lost some accuracy. The calculation for O III [5], performed in a similar manner, does include all the two-body terms of the Breit–Pauli operators but the correlation orbitals, for all the initial and final states include only $4s$, $4p$, $4d$. Thus, no f or g orbitals are present and this also will limit the accuracy.

In the first paper in this series [6], we described a scheme in which orbitals for the initial and final states are optimized separately. Furthermore, configurations associated with groups of terms that mix in the Breit–Pauli approximation, may be optimized simultaneously so as to get an optimal basis for Breit–Pauli interactions. Calculations were performed systematically so that convergence could be monitored and estimates of uncertainty obtained. The scheme was first applied to the Be-like sequence [6] and then the boronlike sequence [7]. As the complexity of the states increases, each system has presented challenges.

In this paper, we extend the approach to the carbonlike sequence by considering all levels up to $2s^22p3d$ $^1P_1^o$, for $Z = 7, \dots, 15$ and up to $2s2p^3$ $^3P_J^o$ in the case of carbon. Lifetimes of levels are reported along with LS uncertainties that are indicators of accuracy. All results are posted at a Web site (see Sect. 3). In addition, in this paper the energy levels and transition data for N II, O III, and Si IX are critically evaluated; energy levels are compared with experiment, transition data reported along with uncertainty estimates, and selected results compared with experiment and recent theory.

2. Computational procedures and optimization strategies

The underlying procedures are the same as those described in the Be-like paper [6] and will not be repeated here.

Briefly, the nonrelativistic multiconfiguration Hartree–Fock (MCHF) approach determines an approximate wave function Ψ for the state labeled γLS of the form

$$\Psi(\gamma LS) = \sum_j c_j \Phi(\gamma_j LS) \quad (2)$$

where γ represents the dominant configuration, and any additional quantum numbers required for uniquely specifying the state being considered. The configuration state functions (CSF) $\{\Phi\}$ are built from a basis of one-electron spin-orbital functions

$$\phi_{nlm_lm_s} = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \varphi) \chi_{m_s} \quad (3)$$

The wave-function expansion is associated with an energy functional for *one* LS term and eigenvalue. The traditional MCHF procedure [8] consists of optimizing to self-consistency *both* the radial functions $\{P_{n_j l_j}(r)\}$ and mixing coefficients $\{c_j\}$ of this energy functional. But in the Breit–Pauli approximation, the wave function for a specific J is an expansion over terms. To obtain a suitable basis for all these terms, the first paper introduced the notion of simultaneous optimization of energy expressions derived from several different terms or even several eigenvalues of the same term. Furthermore, the different energy expressions could be weighted according to importance. The result of such an approach is a basis adequate for simultaneously representing the different terms that mix in a Breit–Pauli approximation.

Systematic, large-scale methods were applied in which the wave-function expansions were obtained from orbital sets of increasing size, allowing for the monitoring of convergence. Our model is best described in terms of a union of sets, whose members satisfy certain rules in the distribution of principal quantum numbers, as in

$$1s \cdot \{1, 2\}^2 \{2, 3, 4\}^3 \cup 1s^2 \{2\} \{2, 3, \dots, n \leq 6\}^2 \cup 1s^2 \{2\}^2 \{2, 3, 4, \dots, n \leq 7\}^2$$

The wave-function expansion includes all possible configuration states from the above distributions of principal quantum numbers. In this notation, the first set includes the effect of core-polarization. It includes all configurations constructed from the $\{1s, 2s, 2p, \dots, 4s, 4p, 4d, 4f\}$ orbital set with at least one $1s$ electron, then two more electrons with either $n = 1$ or 2 , and the remaining three are unrestricted. In the second set, the first two electrons are $1s^2$, the third is either $2s$ or $2p$; the next has a principal quantum number either $n = 2$ or 3 , and the last two electrons have unrestricted principal quantum numbers but with $n \leq 6$. The maximum n (and l) characterize a particular expansion in this model. The $1s$ orbital was obtained from an expansion over $1s \cdot \{1, 2, 3\}^5$ containing all possible configurations from orbitals with $n \leq 3$ and at least one $1s$ orbital. After that, the $1s$ orbital was fixed. For expansions with maximum quantum number $n = 4$ or 5 , all orbitals except $1s$ were varied. For the $n = 6$ calculation, all but $1s, 2s, 2p$ were varied, and for the $n = 7$ calculation, all orbitals with principal quantum number ≥ 5 were varied. In all cases, correlation in $1s^2$ was neglected. Also, all expansions were restricted to $l \leq 6$ or i orbitals. Note that by specifying the expansions by rules that focus on the principal quantum number and include all possible angular quantum numbers, $2s - 2p$ degeneracy effects are automatically included, even though the higher n virtual orbitals are only doubly occupied.

Once a set of radial orbitals has been obtained, the relativistic corrections can be taken into account within the Breit–Pauli approximation by diagonalizing the Breit–Pauli Hamiltonian [8] to get the intermediate coupling wave functions

$$\Psi(\gamma J) = \sum_{LS} \sum_j c_j(LS) \Phi(\gamma_j LSJ) \quad (4)$$

Table 2. Theoretical lifetimes (in s) for excited states up to $2s^22p3d\ ^1P_1^o$ of C-like systems for $Z = 6, \dots, 15$. The notation e-nn is used to denote 10^{nn} .

Term	J	$Z = 6$	$Z = 7$	$Z = 8$	$Z = 9$	$Z = 10$	$Z = 11$	$Z = 12$	$Z = 13$	$Z = 14$	$Z = 15$
$2s2p^3\ ^5S^o$	2	3.436e-02	5.693e-03	1.237e-03	3.455e-04	1.148e-04	4.226e-05	1.869e-05	8.751e-06	4.359e-06	2.292e-06
$2s2p^3\ ^3D^o$	3	7.878e-09	2.679e-09	1.611e-09	1.140e-09	8.698e-10	6.927e-10	5.776e-10	4.932e-10	4.274e-10	3.556e-10
	2	7.868e-09	2.671e-09	1.603e-09	1.131e-09	8.590e-10	6.805e-10	5.637e-10	4.773e-10	4.096e-10	3.755e-10
	1	7.861e-09	2.665e-09	1.598e-09	1.1245e-09	8.522e-10	6.730e-10	5.551e-10	4.677e-10	3.990e-10	3.439e-10
$2s2p^3\ ^3P^o$	2	3.502e-09	7.824e-10	5.382e-10	4.011e-10	3.153e-10	2.565e-10	2.144e-10	1.842e-10	1.603e-10	1.409e-10
	1	3.487e-09	7.837e-10	5.368e-10	3.995e-10	3.135e-10	2.543e-10	2.169e-10	1.871e-10	1.590e-10	1.396e-10
	0	3.479e-09	7.816e-10	5.361e-10	3.987e-10	3.126e-10	2.533e-10	2.133e-10	1.830e-10	1.636e-10	1.446e-10
$2s2p^3\ ^1D^o$	2		3.166e-10	1.813e-09	1.319e-10	1.035e-10	8.462e-11	7.186e-11	6.225e-11	5.461e-11	4.844e-11
$2s2p^3\ ^3S^o$	1		9.305e-11	6.939e-11	5.542e-11	4.585e-11	3.881e-11	3.376e-11	2.980e-11	2.654e-11	2.385e-11
$2s2p^3\ ^1P^o$	1		2.189e-10	9.091e-11	7.314e-11	6.007e-11	5.043e-11	4.357e-11	3.820e-11	3.383e-11	3.022e-11
$2p^4\ ^3P$	2			1.636e-10	1.210e-10	9.413e-11	7.906e-11	6.648e-11	5.722e-11	5.005e-11	4.444e-11
	1			1.634e-10	1.207e-10	9.381e-11	7.867e-11	6.601e-11	5.665e-11	4.937e-11	4.364e-11
	0			1.632e-10	1.206e-10	9.369e-11	7.852e-11	6.584e-11	5.647e-11	4.917e-11	4.343e-11
$2p^4\ ^1D$	2			4.191e-10	2.845e-10	2.077e-11	1.676e-10	1.358e-10	1.133e-10	9.637e-11	8.341e-11
$2p^4\ ^1S$	0				1.641e-10	1.135e-10	8.568e-11	7.029e-11	5.796e-11	4.913e-11	4.255e-11
$2s^22p3s\ ^3P^o$	0	2.778e-09	8.813e-10	2.538e-10	1.085e-10	5.514e-11	3.118e-11	1.924e-11	1.259e-11	8.614e-12	6.100e-12
	1	2.774e-09	7.256e-10	2.534e-10	1.082e-10	5.487e-11	3.094e-11	1.901e-11	1.236e-11	8.385e-12	5.879e-12
	2	2.768e-09	8.777e-10	2.525e-10	1.078e-10	5.467e-11	3.084e-11	1.898e-11	1.237e-11	8.430e-12	5.942e-12
$2s^22p3s\ ^1P^o$	1	2.667e-09	2.189e-10	2.125e-10	7.598e-11	3.657e-11	2.017e-11	1.219e-11	7.850e-12	5.306e-12	3.732e-12
$2s^22p3p\ ^1P$	1			1.532e-07	8.679e-09	3.501e-09	1.810e-09	1.063e-09	6.772e-10	4.547e-10	3.169e-10
$2s^22p3p\ ^3D$	1			1.247e-08	5.326e-09	2.657e-09	1.516e-09	9.311e-10	6.043e-10	4.084e-10	2.840e-10
	2			1.257e-08	5.314e-09	2.649e-09	1.509e-09	9.257e-10	6.000e-10	4.054e-10	2.831e-10
	3			1.209e-08	5.303e-09	2.643e-09	1.506e-09	9.250e-10	6.012e-10	4.083e-10	2.873e-10
$2s^22p3p\ ^3S$	1			6.750e-09	2.362e-09	1.031e-09	5.421e-10	3.175e-10	2.001e-10	1.327e-10	9.137e-11
$2s^22p3p\ ^3P$	0			6.173e-09	2.939e-09	9.084e-10	4.239e-10	2.267e-10	1.332e-10	8.389e-11	5.580e-11
	1			5.961e-09	2.928e-09	9.088e-10	4.248e-10	2.280e-10	1.346e-10	8.563e-11	5.780e-11
	2			5.940e-09	2.912e-09	9.080e-10	4.242e-10	2.272e-10	1.337e-10	8.445e-11	5.638e-11
$2s^22p3p\ ^1D$	2			7.311e-08	3.428e-09	1.647e-09	9.757e-10	6.157e-10	4.048e-10	2.747e-10	1.907e-10
$2s^22p3p\ ^1S$	0			5.363e-08	1.684e-09	9.068e-10	4.832e-10	2.849e-10	1.778e-10	1.157e-10	7.780e-11

Term	<i>J</i>	$Z = 6$	$Z = 7$	$Z = 8$	$Z = 9$	$Z = 10$	$Z = 11$	$Z = 12$	$Z = 13$	$Z = 14$	$Z = 15$
$2s^2 2p3d \ ^1D^o$	2		3.435e-10	1.427e-10	7.698e-11	3.502e-11	1.672e-11	8.977e-12	5.276e-12	3.304e-12	2.161e-12
$2s^2 2p3d \ ^3F^o$	2		6.664e-09	3.202e-10	7.823e-11	3.902e-11	2.429e-11	1.644e-11	1.152e-11	8.256e-12	6.005e-12
	3		7.411e-09	4.105e-09	2.362e-09	1.208e-09	5.506e-10	2.404e-10	1.064e-10	4.912e-11	2.386e-11
	4		8.629e-09	5.160e-09	3.813e-09	3.074e-09	2.607e-09	2.271e-09	2.014e-09	1.823e-09	1.657e-09
$2s^2 2p3d \ ^3D^o$	1		2.280e-10	4.843e-11	1.688e-11	7.544e-12	3.918e-12	2.269e-12	1.416e-12	9.352e-13	6.453e-13
	2		2.293e-10	4.856e-11	1.695e-11	7.604e-12	3.977e-12	2.332e-12	1.481e-12	1.001e-12	7.097e-13
	3		2.289e-10	4.851e-11	1.690e-11	7.544e-12	3.911e-12	2.258e-12	1.403e-12	9.229e-13	6.345e-13
$2s^2 2p3d \ ^3P^o$	2		3.872e-10	8.320e-11	2.918e-11	1.306e-11	6.700e-12	3.781e-12	2.274e-12	1.437e-12	9.488e-13
	1		3.868e-10	8.311e-11	2.918e-11	1.311e-11	6.776e-12	3.877e-12	2.376e-12	1.534e-12	1.032e-12
	0		3.868e-10	8.316e-11	2.925e-11	1.319e-11	6.860e-12	3.963e-12	2.460e-12	1.612e-12	1.102e-12
$2s^2 2p3d \ ^1F^o$	3		2.548e-10	5.014e-11	1.640e-11	6.973e-12	3.488e-12	1.954e-12	1.184e-12	7.617e-13	5.131e-13
$2s^2 2p3d \ ^1P^o$	1		3.685e-10	8.061e-11	2.642e-11	1.125e-11	5.654e-12	3.171e-12	1.924e-12	1.239e-12	8.347e-13

Thus the expansion is now the sum of expansions over a set of terms. For all expansions, the iterative Davidson method [9] was used to determine a few of the lowest eigenvalues and eigenvectors [10].

All the results in this paper, unless specifically stated as being *LS* results, are based on the diagonalization of the Breit–Pauli Hamiltonian in which the orbit–orbit term has been omitted. This operator does not contribute to the mixing of terms, and behaves like a small correlation correction. Experiments in Li-like sequence [11] have shown that inclusion of orbit–orbit can double the computation times for generating the Breit–Pauli interaction matrix, yet have negligible effect at the present level of accuracy. For this reason, it has been omitted, as is common practice. In the rest of the paper, we will refer to our results as MCHF results, and only use MCHF + BP for emphasis, when needed.

The oscillator strengths f are calculated using the standard, nonrelativistic operators for length and velocity forms (see ref. 6 for details). The nonrelativistic line strengths allow us to monitor the convergence between the two forms with the improvement of the wave functions. In the Breit–Pauli approximation, the same length form is correct to $O(\alpha^2)$ while the velocity form requires a relativistic correction to the gradient operator [12]. For this reason, it is customary to report both length and velocity results for an *LS* calculation, but only the length form in the Breit–Pauli calculation. No orthonormality constraints are imposed *between* the two sets of radial functions spanning the total wave functions of the initial and final state, allowing *separate* MCHF optimizations for the two states involved.

The different states of the C-like ions were grouped together and a radial basis determined for a set of terms and (or) eigenvalues that were deemed to be important for the relativistic effects. In Table 1, on the left are the group of terms for which accurate Breit–Pauli results are required. But because these may mix with additional terms, the latter are listed in the second group. Sometimes these are different eigenfunctions of the same terms and this is indicated by the configuration. Mixing with some of the terms may not be particularly strong. In such cases these *LS* eigenstates had a smaller weight as indicated in Table 1. The neutral atom has a somewhat different spectrum. States with $4s$ lie much lower in the spectrum and $2p^4$ much higher. A study of carbon going as high as the $1s^22s^22p6s$ will be undertaken as a separate investigation.

3. Breit–Pauli results

The orbital basis from simultaneous optimization may be used to determine J -dependent energy levels and transition rates. In Table 2 we report the lifetimes of all the levels of the configurations considered in this work. These are based on the allowed E1 transitions.

A complete set of transition data (transition energies, line strength, oscillator strengths, transition rates) is available at

http://www.vuse.vanderbilt.edu/~cff/mchf_collection

This site also reports *LS* convergence trends, including the length and velocity forms of the line strength. As shown in our earlier paper [6] the latter can be used in the estimation of accuracy. All other reported data are based on Breit–Pauli line strengths in the length form. For each atom or ion, an ascii file may be viewed or downloaded; the file contains all the information about the transitions in floating point form, suitable for processing.

The rest of this paper is devoted to the critical evaluation of results for selected members of the isoelectronic sequence.

4. Accuracy of Breit–Pauli energies

One measure of accuracy, generally the easiest to evaluate, is the accuracy of the spectra produced by the calculations. Table 3 compares the present ab initio spectra with observation for N II, O III, and Si IX. Because of the lack of experimental data, not as many comparisons are possible for Si IX, but we note the relatively larger error in the excitation energy for $2s2p^3$ levels. A similar error was not

Table 3. Comparison of the computed spectrum for N II, O III, and Si IX with tabulated NIST [21] data.

Config.	LS	J	N II			O III			Si IX		
			Theory	Obs.	Diff.	Theory	Obs.	Diff.	Theory	Obs.	Diff.
$2s^2 2p^2$	3P	0									
	1	48.9	48.7	0.2		113.4	113.2	0.2	2582	2545	37
	2	130.7	130.8	-0.1		305.6	306.2	-0.6	6452	6414	38
	1D	2	15405.6	15316.2	89.4	20369.4	20273.3	96.1	53076	52926	150
	1S	0	32848.8	32688.8	160.0	43278.1	43185.7	92.4	107826	107799	27
$2s 2p^3$	$^5S^o$	2	46714.3	46784.6	-70.3	60531.6	60324.8	206.8	154077	150770	3307
	$^3D^o$	3	92348.6	92237.2	111.4	120464.4	120025.2	439.2	296224	292232	3992
	2	92362.2	92250.3	111.8		120492.2	120053.4	438.8	296274	292296	3978
	1	92363.4	92251.8	111.6		120497.7	120058.2	439.5	296405	292441	3964
	$^3P^o$	0	109415.0	109216.6	198.4	142919.3	142393.5	525.8	348103	344075	4028
	1	109414.5	109217.6	196.9		142905.3	142381.8	523.5	348047	344009	4038
	2	109421.6	109223.5	198.1		142903.3	142381.0	522.3	348157	344118	4039
	$^1D^o$	2	144516.0	144187.9	328.0	187666.3	187054.0	612.3	444583	440403	4179
	$^3S^o$	1	155386.3	155126.7	259.5	197581.2	197087.7	493.5	450039	446942	4097
	$^1P^o$	1	167411.1	166765.7	645.4	211184.4	210461.8	722.6	497004	492755	4249
$2p^4$	3P	2				284695.5	283759.7	935.8	675134	674764	370
	1					284911.5	283977.4	934.1	679689	679300	389
	0					285005.6	284071.9	933.7	681455	681079	376
	1D	2				299391.6	298294.0	1097.6	720026	719502	524
	1S	0				344761.7	343306.3	1455.4	820335	819689	646
$2s^2 2p3s$	$^3P^o$	0	149178.5	149076.5	102.0	267842.0	267258.7	583.3	1623869		
	1	149044.1	148940.2	104.0		267960.1	267377.1	583.0	1625527	1623380	2147
	2	149011.0	148908.6	102.4		268216.0	267634.0	582.0	1630766	1628500	2266
	$^1P^o$	1	149308.3	149187.8	120.5	273720.2	273081.3	638.8	1643254.	1640850	2405
$2s^2 2p3p$	1P	1	165108.9	164610.8	498.1	291672.6	290958.3	714.4	1697991		
	3D	1	167165.0	166678.6	486.4	294577.4	293866.5	710.9	1705325		
	2	167069.3	166582.5	486.9		294712.8	294002.9	710.0	1707004		
	3	167008.8	166521.7	487.1		294931.6	294223.1	708.5	1711479		
	3S	1	169359.1	168892.2	466.9	298229.4	297558.7	670.7	1718810		
	3P	0	171192.6	170666.2	526.8	300907.2	300239.9	667.3	1723186		
	1	171134.5	170607.9	526.8		300988.7	300312.0	676.7	1725617		
	2	171099.5	170572.6	526.9		301118.1	300442.6	675.6	1727634		
	1D	2	174744.1	174212.0	532.1	307322.0	306586.1	735.9	1750579		
	1S	0	178901.2	178273.4	627.8	314671.4	313802.8	868.6	1778071		
$2s^2 2p3d$	$^3F^o$	2	187095.8	186511.6	584.2	325112.6	324464.9	647.7	1792022		
	3	187155.1	186571.0	584.1		325312.8	324660.8	652.0	1795571		
	4	187236.8	186652.4	584.3		325490.7	324839.0	651.7	1799198		
	$^1D^o$	2	187666.8	187091.4	575.4	325374.6	324735.7	639.0	1796778	1794050	2728
	$^3D^o$	1	187976.5	187437.6	538.9	327828.1	327229.3	598.8	1810903	1808160	2743
	2	188000.7	187461.6	539.1		327877.0	327278.3	598.7	1811773	1809040	2733
	3	188030.7	187491.9	538.8		327950.4	327352.2	598.3	1814103	1811430	2673
	$^3P^o$	2	189421.6	188857.4	564.2	330077.9	329469.8	608.1	1818302	1815650	2652
	1	189474.2	188909.2	565.0		330192.2	329583.9	608.3	1819504	1816900	2604
	0	189502.6	188937.2	565.4		330253.8	329645.1	608.6	1820192	1817630	2562
	$^1F^o$	3	189876.2	189335.2	541.0	332452.6	331821.4	631.1	1840609	1837780	2829
	$^1P^o$	1	190765.9	190120.2	645.7	333420.7	332778.9	641.7	1841316	1838560	2756

Table 4. Comparison of the present computed and observed (NIST) fine-structure splitting (in cm^{-1}) relative to the lowest level of the observed multiplet. In the case of Si IX, the differences from the observed and the earlier Breit–Pauli calculations [22] are given in parentheses.

Config.	LS	J	N II			O III			Si IX		
			Theory	Obs.	Diff.	Theory	Obs.	Diff.	Theory	Obs.	Diff.
$2s^22p^2$	3P	0									
		1	48.87	48.7	0.2	113.37	113.18	0.19	2583	2545	37(–6)
		2	130.72	130.8	–0.1	305.60	306.17	–0.57	6452	6414	38(–2)
	$^3D^o$	3									
		2	13.52	13.1	0.42	27.79	28.20	–0.41	50	64	–14(3)
		1	14.7	14.6	0.10	33.29	33.00	0.29	181	209	–28(6)
$2s^22p3s$	$^3P^o$	2							110	109	1(–7)
		1	0.52	1.52	–1.0	1.99	0.80	1.19			
		0	7.07	5.90	1.17	15.96	12.50	3.46	56	66	–10(–15)
	$^3P^o$	2									
		1	33.17	31.58	1.59	118.03	118.40	–0.3			
		2	167.56	167.93	0.37	374.02	375.29	–1.27			
$2s^22p3p$	3D	3									
		2	60.47	60.76	–0.29	135.46	136.37	–0.91			
		1	156.21	156.95	–0.74	354.19	356.58	–2.39			
	3P	2									
		1	35.03	35.28	–0.25	81.48	72.03	9.45			
		0	93.11	93.62	–0.51	210.94	202.62	8.3			

observed for $2s2p^2$ in our B-like results for Si X [7]. We note an almost uniform error for the terms of this configuration, suggesting a common cause, probably related to the model used. Term mixing will be most important for the levels of $2s^22p3d$. We note a relatively small variation of the errors in each spectrum, implying that a simple energy shift will not dramatically change the mixing of terms. By comparison, the variation in term energies in earlier CIV3 calculations was much larger [5, 13, 14], not to mention the errors themselves.

In Table 4 some of the present fine-structure splittings are compared with observation. The largest relative discrepancy between theory and observation is for the levels of the $2s2p^3\ ^3P^o$ term. This is a case where the order of the levels changes as the atomic number increases with the $J = 1$ level becoming the lowest. The fine-structure splitting for the ground state is more than an order of magnitude more accurate in our present work than in the earlier CIV3 calculations [5, 13, 14].

5. Accuracy of Breit–Pauli transitions

Ab initio Breit–Pauli transition rates contain errors arising mainly from neglected correlation and incorrect mixing of terms. The discrepancy in length and velocity forms of the line strength (or gf-value) has a similar origin as neglected correlation. As shown in our earlier paper [6], the agreement in length and velocity forms of the line strength can be used in the estimation of accuracy. Since C-like, is considerably more complex than B-like, we have introduced a somewhat different definition of this factor. The relative discrepancy, δS (as a fraction), is defined as

$$\delta S = |S_l - S_v| / \max((S_l, S_v))$$

It might appear that the difference should be relative to the average of S_l and S_v , but when there is cancellation in the line strength and the two differ by an order of magnitude, the above assures that the error is never greater than 100%.

Table 5. Difference between S_v and S_l in % for allowed singlet–singlet and triplet–triplet transitions.

Transition		6	7	8	9	10	11	12	13	14	15	
$2p^2$	3P – $2s2p^3$	$^3D^o$	0.36	1.04	0.75	0.25	0.78	0.90	0.91	1.24	1.15	
	3P –	$^3P^o$	0.46	0.19	0.083	0.28	1.13	1.17	1.13	1.35	1.25	
	3P –	$^3S^o$	0.29	0.12	0.28	0.73	1.31	1.34	1.29	1.44	1.30	
	3P – $2p3s$	$^3P^o$	8.64	3.13	2.69	1.83	1.26	1.43	1.16	0.86	0.40	0.088
	3P – $2p3d$	$^3D^o$	1.96	1.51	1.06	1.03	1.10	0.90	0.66	0.57	0.44	
	3P –	$^3P^o$	1.77	1.52	1.07	1.05	1.08	0.90	0.66	0.58	0.46	
	1D – $2s2p^3$	$^1D^o$	0.33	0.013	0.14	0.60	1.28	1.31	1.26	1.45	1.32	
	1D –	$^1P^o$	1.47	0.29	0.39	0.73	1.33	1.33	1.27	1.41	1.28	
	1D – $2p3s$	$^1P^o$	4.75	0.32	1.24	0.99	1.17	0.75	0.59	0.53	0.56	0.58
	1D – $2p3d$	$^1D^o$	0.18	0.49	0.51	0.34	0.20	0.18	0.31	0.23	0.24	
	1D –	$^1F^o$	0.52	0.033	0.091	0.21	0.39	0.35	0.24	0.23	0.17	
	1D –	$^1P^o$	73.35	13.21	9.23	7.25	6.20	5.30	4.76	3.85	3.30	
	1S – $2s2p^3$	$^1P^o$	0.94	0.26	0.27	0.84	1.55	1.58	1.51	1.70	1.54	
	1S – $2p3s$	$^1P^o$	4.92	10.36	3.31	2.98	2.93	2.62	2.17	1.84	1.67	1.45
	1S – $2p3d$	$^1P^o$	1.54	1.64	1.03	0.75	0.51	0.34	0.35	0.25	0.23	
$2s2p^3$	$^3D^o$ – $2p^4$	3P	0.43	0.30	0.13	1.26	1.01	0.87	0.99	1.00		
	$^3D^o$ – $2p3p$	3D	9.36	1.90	3.78	4.48	4.68	4.60	4.41	4.18	3.73	
	$^3D^o$ –	3P	7.65	5.96	4.97	4.75	4.39	3.95	3.50	3.12	2.68	
	$^3P^o$ – $2p^4$	3P	0.40	0.000	0.42	3.33	3.24	3.08	2.45	2.43		
	$^3P^o$ – $2p3p$	3D	2.29	1.94	1.27	0.43	1.02	1.03	0.84	0.67	0.53	
	$^3P^o$ –	3S	6.77	3.53	4.04	3.54	3.21	2.98	2.80	2.62	2.28	
	$^3P^o$ –	3P	10.45	13.17	15.85	15.03	13.15	11.05	9.20	7.77	6.36	
	$^1D^o$ – $2p^4$	1D	0.55	0.27	0.011	2.39	2.04	1.76	1.65	1.62		
	$^1D^o$ – $2p3p$	1D	2.07	35.46	16.65	12.98	10.58	8.71	7.16	6.00	5.09	
	$^3S^o$ – $2p^4$	3P	0.48	0.13	0.13	3.05	2.59	2.26	2.10	2.04		
	$^3S^o$ – $2p3p$	3P	57.12	25.04	24.84	13.52	9.15	6.64	4.78	3.59	3.09	
	$^1P^o$ – $2p^4$	1D	0.52	0.064	0.66	5.13	4.99	4.68	3.55	3.48		
	$^1P^o$ –	1S	0.99	0.52	0.22	1.05	0.39	0.044	0.90	0.80		
	$^1P^o$ – $2p3p$	1D	8.50	10.91	6.82	0.40	2.56	3.33	3.19	2.81	2.59	
	$^1P^o$ –	1S	54.30	16.36	15.75	9.51	6.56	5.05	4.09	3.48	2.95	
$2p^4$	3P – $2p3s$	$^3P^o$	18.56	67.14	50.24	46.53	37.03	31.15	20.24	17.51		
	3P – $2p3d$	$^3D^o$	11.42	62.11	81.99	42.84	86.76	100.0	85.16	82.61		
	3P –	$^3P^o$	0.32	38.43	20.42	28.36	38.34	41.72	11.07	15.93		
	1D – $2p3s$	$^1P^o$	5.00	99.26	77.63	28.62	85.49	96.06	88.45	96.03		
	1D – $2p3d$	$^1D^o$	98.90	9.02	8.79	19.31	8.42	7.68	18.35	16.68		
	1D –	$^1F^o$	5.33	56.56	40.88	3.19	12.36	12.82	6.45	4.64		
	1D –	$^1P^o$	11.25	96.01	79.99	16.13	49.85	45.27	38.32	27.13		
	1S – $2p3s$	$^1P^o$	7.04	99.61	97.98	99.94	99.77	99.52	99.85	94.35		
	1S – $2p3d$	$^1P^o$	76.39	75.03	57.94	75.22	79.72	82.06	45.71	50.13		
$2p3s$	$^3P^o$ – $2p3p$	3D	6.98	3.32	4.42	4.00	3.12	2.52	2.11	1.87	1.60	
	$^3P^o$ –	3S	12.38	7.76	7.72	6.70	5.93	5.10	4.39	4.03	4.07	
	$^3P^o$ –	3P	4.57	2.03	3.15	2.72	2.01	1.54	1.23	0.67	0.36	
	$^1P^o$ –	1D	5.72	1.97	3.27	3.26	2.48	2.02	1.77	1.89	1.37	
	$^1P^o$ –	1S	7.19	7.09	6.46	5.26	4.59	3.84	3.24	2.67	2.53	
$2p3p$	3D – $2p3d$	$^3F^o$	2.55	1.11	0.82	1.32	1.06	0.54	0.49	0.028	0.20	
	3D –	$^3D^o$	4.41	0.044	0.74	1.36	1.91	2.96	1.55	3.27	2.53	
	3D –	$^3P^o$	35.11	22.18	21.09	19.42	18.49	14.57	14.74	13.30	12.93	
	3S –	$^3P^o$	2.09	1.55	1.92	2.38	2.69	2.72	2.18	2.88	2.49	
	3P –	$^3D^o$	6.76	1.04	0.010	0.032	0.55	1.12	1.08	1.47	1.37	
	3P –	$^3P^o$	10.77	1.47	0.38	1.72	1.45	0.30	0.61	1.51	1.01	
	1D –	$^1D^o$	19.87	11.89	9.52	7.44	5.38	3.00	3.95	1.72	2.06	
	1D –	$^1F^o$	10.93	2.12	0.62	0.31	0.79	0.84	1.28	0.93	1.19	
	1D –	$^1P^o$	41.01	30.18	31.44	28.14	26.64	22.83	24.27	21.62	21.32	
	1S –	$^1P^o$	16.48	5.57	2.58	0.81	2.20	2.32	2.39	2.25	2.71	

Table 5 displays the discrepancies (in %) for singlet–singlet and triplet–triplet transitions along the isoelectronic sequence. This table gives an indication of the accuracy of all the data and not just the spectra evaluated here. Note that for most transitions the discrepancy decreases with increasing Z , that there is a large difference between the various line strength accuracies.

Many transitions depend crucially on the mixing of terms, mixing that is sensitive to the separation of term energies of a configuration. To improve the transition rate, term energy corrections to the Breit–Pauli interaction matrix were applied, where all the diagonals of a given term are shifted by an amount equal to the difference between the ab initio energy and observed. This brings the adjusted spectrum (displayed at the Web site) within 1–2 cm^{-1} of observed. The change in the transition rates from this adjustment is another indicator of accuracy but this is more difficult to evaluate without actually performing calculations, in general.

It is not at all obvious how an uncertainty should be estimated but in this work, we have applied what in most cases (not all) is a generally conservative formula. The tables presented here are adjusted values to improve accuracy (see ref. 6 for more details). Let A' be the value of A adjusted for the observed transition energy, a process that assumes that the line strength may be accurate but the transition energy may be in error. In such circumstances this “normalization” improves the accuracy. To improve the Breit–Pauli mixing, adjustments were made to the diagonal energies of terms. This also is a form of normalization. Let the resulting transition rates be A'' . Also let, δe be the relative error in the transition energy. For allowed transitions, we have defined the δS to be the LS discrepancy for that transition which is equivalent to assuming term mixing is negligible. For an intercombination line, the line strength comes from term mixing either in the initial or final state, or both. To process a large number of transitions and obtain δS automatically from LS uncertainties, the following assumptions were made: (i) that only terms of the same configuration mix, and (ii) that all mixing was equally likely. Consequently, for an intercombination transition from configuration γ to γ' with terms $L_i S_i$ and $L'_{i'} S'_{i'}$, respectively, we assumed

$$\delta S = \sum_i \sum_{i'} \delta S(L_i S_i, L'_{i'} S'_{i'}) / N \quad (5)$$

where $\delta S(L_i S_i, L'_{i'} S'_{i'})$ is the relative error in the line strength for an LS transition between the indicated terms, and N is a normalization factor equal to the number of nonzero line strengths.

Then the uncertainty was defined as

$$|A' - A''| + (\delta e + \delta S) A'' \quad (6)$$

It can be argued that the quantity $|A' - A''|$ should not be included in that the adjustment has *improved* the transition rate, like in the $2s^2 \ ^1S_0 - 2s2p \ ^3P_1^o$ [6,8], where the adjustment process makes certain that the singlet–triplet mixing is correct. Definitely, the adjustment improves the transition rate. But it can also be argued, that agreement in the length and velocity forms of the line strength is not a good criterion in that the length form is the more reliable. But cases have also been encountered where length and velocity forms agreed well but changed by more than their difference as the correlation model changed. When the uncertainty is large due to the discrepancy in the line strength, it may well be that the uncertainty is too large. At the same time, when two J levels are extremely close, there may be a large change $|A' - A''|$ with A'' being more accurate than the formula implies.

Table 6 presents critically evaluated transition data along with uncertainties in their values. The uncertainty (in parentheses) is usually given in terms of the last decimal place given. Thus 5.08(20) implies 5.08 ± 0.20 whereas 9.097(45) implies 9.097 ± 0.045 . To conserve space, occasionally the uncertainty is given in %.

It should be mentioned, that at the Web site, the spectrum .lsj file includes results in both length and velocity form, but the velocity form operator has neglected some of the relativistic corrections which may be important, particularly for an intercombination line. In many cases, the agreement is excellent, as

Table 6. Present adjusted transition rates (in s⁻¹) and uncertainties (in parentheses) for N II, O III, and Si IX. See the text for a discussion of the interpretation of “uncertainty.”

Multiplet		N II		O III		Si IX	
Lower	Upper	Present	x	Present	x	Present	x
2p ²	³ P ₀	2s2p ³	³ D ₁ ^o	2.095(9)	8	3.489(42)	8
			³ P ₁ ^o	4.226(22)	8	6.112(22)	8
			³ S ₁ ^o	1.189(4)	9	1.588(3)	9
			¹ P ₁ ^o	1.023(156)	4	6.279(491)	4
	² p3s		³ P ₁ ^o	3.401(153)	8	1.307(35)	9
			¹ P ₁ ^o	3.796(600)	7	7.012(370)	5
	² p3d		³ D ₁ ^o	2.460(52)	9	1.194(19)	10
			³ P ₁ ^o	7.171(137)	8	3.277(50)	9
			¹ P ₁ ^o	3.937(474)	6	1.568(55)	7
			⁵ S ₂ ^o	5.155(66)	1	2.308(37)	2
³ P ₁	2s2p ³		³ D ₂ ^o	2.823(12)	8	4.693(57)	8
			³ D ₁ ^o	1.545(7)	8	2.542(31)	8
			³ P ₂ ^o	3.139(15)	8	4.506(15)	8
			³ P ₁ ^o	3.214(17)	8	4.706(18)	8
			³ P ₀ ^o	1.273(7)	9	1.846(7)	9
			¹ D ₂ ^o	5.657(564)	3	1.325(79)	4
			³ S ₁ ^o	3.565(13)	9	4.765(10)	9
			¹ P ₁ ^o	1.694(46)	5	8.959(427)	5
			³ P ₀ ^o	1.134(37)	9	3.922(117)	9
			³ P ₁ ^o	2.530(113)	8	9.791(276)	8
² p3s	² p3d		³ P ₂ ^o	2.842(94)	8	9.822(284)	8
			¹ P ₁ ^o	3.019(452)	7	9.319(854)	5
			³ F ₂ ^o	6.404(674)	6	3.405(360)	6
			¹ D ₂ ^o	2.622(539)	7	3.448(128)	7
			³ D ₁ ^o	1.701(33)	9	8.002(121)	9
			³ D ₂ ^o	3.289(76)	9	1.608(26)	10
			³ P ₂ ^o	4.834(89)	8	2.091(35)	9
			³ P ₁ ^o	6.856(131)	8	3.424(55)	9
			³ P ₀ ^o	2.443(43)	9	1.172(18)	10
			¹ P ₁ ^o	8.74(139)	4	1.170(80)	6
³ P ₂	2s2p ³		⁵ S ₂ ^o	1.266(16)	2	5.765(82)	2
			³ D ₃ ^o	3.721(16)	8	6.138(74)	8
			³ D ₂ ^o	9.097(41)	7	1.478(18)	8
			³ D ₁ ^o	9.963(46)	6	1.603(19)	7
			³ P ₂ ^o	9.548(50)	8	1.387(5)	9
			³ P ₁ ^o	5.272(29)	8	7.608(30)	8
			¹ D ₂ ^o	4.141(128)	4	2.810(55)	5
			³ S ₁ ^o	5.940(22)	9	7.948(18)	9
			¹ P ₁ ^o	3.149(491)	4	1.947(157)	5
			³ P ₁ ^o	4.375(178)	8	1.635(49)	9
² p3s	² p3d		³ P ₂ ^o	8.521(272)	8	2.945(80)	9
			¹ P ₁ ^o	3.683(573)	7	7.438(372)	5
			³ F ₂ ^o	2.350(227)	6	9.165(197)	6
			³ F ₃ ^o	1.521(161)	7	4.077(117)	7
			¹ D ₂ ^o	6.288(75%)	5	2.068(86%)	4
³ P ₁	² s2p ³		³ D ₁ ^o	9.544(228)	7	4.178(73)	8
			³ D ₂ ^o	9.349(195)	8	4.231(68)	9

Table 6. (continued)

Multiplet		N II		O III		Si IX	
Lower	Upper	Present	x	Present	x	Present	x
$2p^2$	3P_2	$2p3d$	${}^3D_3^o$	4.243(89)	9	2.033(32)	10
			${}^3P_2^o$	1.959(39)	9	9.638(157)	9
			${}^3P_1^o$	1.040(19)	9	5.028(78)	9
			${}^1F_3^o$	1.856(32)	6	4.854(132)	6
			${}^1P_1^o$	5.909(903)	5	1.371(55)	6
	1D_2	$2s2p^3$	${}^5S_2^o$	8.948(345)	4	5.777(250)	3
			${}^3D_3^o$	4.140(115)	3	2.108(62)	4
			${}^3D_2^o$	7.330(347)	2	4.093(57)	3
			${}^3D_1^o$	5.928(369)	2	2.358(71)	3
			${}^3P_2^o$	2.297(188)	3	7.088(449)	3
$2p3s$			${}^3P_1^o$	5.158(424)	3	2.746(73)	4
			${}^1D_2^o$	3.143(14)	9	5.463(8)	9
			${}^3S_1^o$	1.056(181)	5	3.093(191)	5
			${}^1P_1^o$	3.167(47)	9	9.380(41)	9
			${}^3P_1^o$	3.806(557)	8	1.890(275)	6
			${}^3P_2^o$	7.17(278)	3	1.890(346)	5
			${}^1P_1^o$	3.693(59)	9	3.023(38)	9
	2p3d		${}^3F_2^o$	2.352(96)	7	2.723(211)	9
			${}^3F_3^o$	2.318(68)	6	8.134(554)	6
			${}^1D_2^o$	2.735(12)	9	6.916(216)	9
1S_0	$2s2p^3$		${}^3D_1^o$	7.08(393)	2	4.768(441)	5
			${}^3D_2^o$	1.378(368)	7	3.044(335)	6
			${}^3D_3^o$	1.387(46)	6	4.107(167)	6
			${}^3P_2^o$	3.232(89)	6	1.022(25)	7
			${}^3P_1^o$	3.272(414)	4	7.51(297)	3
			${}^1F_3^o$	3.830(22)	9	1.971(1)	10
			${}^1P_1^o$	4.239(74%)	5	2.862(379)	8
			${}^3D_1^o$	3.619(43)	2	1.699(16)	3
			${}^3P_1^o$	2.057(30)	3	9.578(109)	3
			${}^3S_1^o$	1.851(117)	4	6.975(419)	4
$2p3s$	$2p3d$		${}^1P_1^o$	1.346(16)	9	1.508(6)	9
			${}^3P_1^o$	2.650(396)	6	1.029(52)	6
			${}^1P_1^o$	2.564(333)	7	1.647(55)	9
			${}^3D_1^o$	1.426(145)	6	5.984(207)	6
			${}^3P_1^o$	2.302(326)	6	6.389(242)	6
			${}^1P_1^o$	2.583(42)	9	1.180(20)	10
	$2s2p^3$	${}^5S_2^o$	3P_1			7.841(112)	3
			3P_2			1.994(28)	4
			1D_2			7.54(105)	1
	$2p3p$		1P_1	2.899(217)	2	4.49(246)	4
$2p3p$			3D_1	3.042(219)		2.603(128)	1
			3D_2	2.416(162)	1	2.005(117)	2
			3D_3	8.127(410)	1	6.559(206)	2
			3S_1	2.306(165)	2	2.220(110)	3
			3P_1	2.905(263)		4.507(176)	1
			3P_2	1.393(88)	1	5.552(275)	1
			1D_2	9.649(649)	3	2.332(150)	1
	${}^3D_3^o$	$2p^4$	3P_2			4.080(19)	9
			1D_2			5.398(598)	5
						7.166(123)	7

Table 6. (continued)

Multiplet		N II		O III		Si IX			
Lower	Upper	Present	x	Present	x	Present	x		
$2s2p^3$	${}^3D_3^o$	$2p3p$	3D_2	1.271(122)	6	5.602(109)	6	3.31(143)	8
			3D_3	6.397(610)	6	2.923(56)	7	9.733(368)	8
			3P_2	5.105(405)	7	1.099(73)	8	9.03(383)	9
			1D_2	1.207(103)	4	6.515(425)	4	1.003(432)	8
${}^3D_2^o$	$2p^4$		3P_1			3.635(17)	9	1.049(16)	10
			3P_2			7.419(36)	8	2.624(31)	9
			1D_2			1.052(86)	5	1.372(41)	7
	$2p3p$	1P_1	1.302(398)	1	8.369(480)	3	2.223(72%)	6	
${}^3D_2^o$	$2p3p$	3D_1	1.940(186)	6	8.684(169)	6	3.74(262)	8	
		3D_2	4.902(466)	6	2.266(44)	7	6.424(248)	8	
		3D_3	7.547(716)	5	3.380(64)	6	7.96(256)	7	
		3S_1	6.743(805)	4	2.570(126)	5	7.42(503)	8	
		3P_1	4.538(359)	7	9.664(651)	7	6.27(434)	9	
		3P_2	9.334(743)	6	2.010(134)	7	2.260(63)	9	
		1D_2	3.920(212)	2	1.080(103)	3	6.364(218)	6	
${}^3D_1^o$	$2p^4$	3P_0			4.857(22)	9	1.424(20)	10	
		3P_1			1.227(5)	9	3.989(51)	9	
		3P_2			5.013(25)	7	2.048(21)	8	
		1D_2			9.91(480)	1	4.061(192)	5	
		1S_0			1.205(296)	4	3.518(71)	6	
$2p3p$		1P_1	7.071(470)	3	5.201(212)	4	1.536(41)	8	
		3D_1	5.284(503)	6	2.439(47)	7	5.226(205)	8	
		3D_2	1.027(97)	6	4.660(89)	6	1.525(665)	8	
		3S_1	2.320(277)	4	9.046(448)	4	4.709(165)	8	
		3P_0	6.076(482)	7	1.289(86)	8	5.316(99%)	9	
		3P_1	1.537(122)	7	3.275(220)	7	3.481(95)	9	
		3P_2	6.318(503)	5	1.360(90)	6	2.40(102)	8	
		1D_2	1.047(94)	2	3.400(334)	2	2.77(118)	6	
		1S_0	8.41(122)	3	5.340(699)	4	5.351(99%)	7	
${}^3P_2^o$	$2p^4$	3P_1			3.293(27)	8	2.052(64)	9	
		3P_2			5.570(43)	8	2.383(74)	9	
		1D_2			3.083(99%)	2	1.128(66)	6	
$2p3p$		1P_1	3.054(212)	3	5.175(268)	4	3.23(221)	7	
		3D_1	5.971(138)	5	1.686(33)	6	1.015(678)	8	
		3D_2	5.398(126)	6	1.458(28)	7	5.201(28)	8	
		3D_3	2.215(52)	7	5.813(114)	7	2.852(828)	9	
		3S_1	4.390(299)	7	1.666(59)	8	3.37(232)	9	
		3P_1	1.975(227)	6	2.849(400)	6	1.491(70%)	7	
		3P_2	2.394(253)	6	9.67(132)	6	1.224(84)	9	
		1D_2	1.501(143)	1	6.801(417)	3	1.006(30)	7	
${}^3P_1^o$	$2p^4$	3P_0			7.711(62)	8	4.165(124)	9	
		3P_1			1.819(14)	8	6.571(195)	8	
		3P_2			1.903(14)	8	9.729(278)	8	
		1D_2			1.848(188)	4	6.680(394)	6	
		1S_0			7.913(335)	4	2.096(33)	7	
$2p3p$		1P_1	2.476(169)	4	1.391(64)	5	2.306(63)	8	
		3D_1	9.074(213)	6	2.380(46)	7	5.158(31)	8	
		3D_2	1.667(39)	7	4.308(85)	7	2.339(946)	9	
		3S_1	2.701(186)	7	9.667(344)	7	2.457(63)	9	

Table 6. (continued)

Multiplet		N II		O III		Si IX	
Lower	Upper	Present	x	Present	x	Present	x
$2s2p^3$	${}^3P_1^o$	$2p3p$	3P_0	3.213(340)	6	1.303(180)	7
			3P_1	5.169(640)	5	5.060(689)	6
			3P_2	7.032(755)	5	3.714(511)	6
			1D_2	1.594(111)	3	1.484(105)	3
			1S_0	9.99(155)	1	4.821(586)	3
	${}^3P_0^o$	$2p^4$	3P_1			2.523(19)	8
		$2p3p$	1P_1	4.059(226)	3	3.233(111)	4
			3D_1	1.233(29)	7	3.178(62)	7
			3S_1	9.086(628)	6	3.151(112)	7
			3P_1	7.929(915)	5	5.932(814)	6
${}^1D_2^o$	$2p^4$		3P_1			1.552(75)	3
			3P_2			9.863(316)	4
			1D_2			2.164(13)	9
	$2p3p$		1P_1	3.041(185)	6	5.682(220)	7
			3D_1	3.399(226)	3	1.214(52)	5
			3D_2	5.85(132)		4.491(357)	3
			3D_3	1.203(111)	2	2.807(67)	2
			3S_1	1.441(116)	3	3.130(155)	4
			3P_1	2.088(404)	1	4.001(196)	3
			3P_2	6.606(515)	2	7.68(253)	4
${}^3S_1^o$	$2p^4$		1D_2	2.011(50)	6	7.02(263)	6
			3P_0			4.377(35)	8
			3P_1			4.357(35)	8
			3P_2			4.313(34)	8
			1D_2			5.63(211)	2
			1S_0			9.342(284)	5
	$2p3p$		1P_1	4.173(376)	2	3.000(315)	3
			3D_1	2.059(72%)	2	5.479(411)	2
			3D_2	1.356(149)		1.190(99)	3
			3S_1	1.418(155)	1	2.249(163)	3
${}^1P_1^o$	$2p^4$		3P_0	1.132(661)	4	9.90(273)	5
			3P_1	1.170(683)	4	9.53(263)	5
			3P_2	1.222(714)	4	8.81(243)	5
			1D_2	3.164(344)	3	1.228(123)	4
			1S_0	5.588(952)	3	4.262(616)	4
			3P_0			8.458(573)	3
			3P_1			3.590(189)	4
			3P_2			1.465(66)	4
			1D_2			1.851(22)	8
			1S_0			5.921(104)	9
$2p3p$	$2p^4$		1P_1			2.612(108)	7
			3D_1			5.333(242)	4
			3D_2			8.715(592)	3
			3S_1	4.069(373)		9.758(537)	3
			3P_0	1.006(130)		3.177(416)	4
			3P_1	6.480(413)		5.163(339)	2
			3P_2	8.621(725)		7.315(75%)	2
			1D_2	6.341(561)	5	6.837(751)	7
			1S_0	1.158(634)	6	2.289(375)	8

Table 6. (continued)

Multiplet		N II		O III		Si IX	
Lower	Upper	Present	x	Present	x	Present	x
$2p^4$	3P_0	${}^3P_1^o$				6.67(163)	5
		${}^1P_1^o$				6.856(99%)	4
	$2p3d$	${}^3D_1^o$		5.94(202)	5	5.242(99%)	3
		${}^3P_1^o$		1.881(381)	5	9.65(158)	6
		${}^1P_1^o$		8.16(156)	2	6.70(159)	3
	3P_1	${}^3P_0^o$				2.171(494)	6
		${}^3P_1^o$				5.76(148)	5
		${}^3P_2^o$				5.52(227)	5
		${}^1P_1^o$				8.09(486)	4
	$2p3d$	${}^3F_2^o$		1.564(269)	2	1.881(771)	4
3P_1		${}^1D_2^o$		2.31(116)	3	5.28(263)	4
		${}^3D_1^o$		3.90(130)	5	1.616(86%)	6
		${}^3D_2^o$		7.96(268)	5	6.970(99%)	4
		${}^3P_2^o$		1.244(263)	5	7.81(136)	6
	$2p3d$	${}^3P_1^o$		1.874(354)	5	5.69(131)	6
		${}^3P_0^o$		6.50(124)	5	2.422(388)	7
		${}^1P_1^o$		3.835(99%)	1	3.26(115)	5
	$2p3s$	${}^3P_1^o$				9.01(253)	5
		${}^3P_2^o$				1.954(539)	6
		${}^1P_1^o$				1.95(134)	4
3P_2	$2p3d$	${}^3F_2^o$		4.02(169)	2	1.509(394)	5
		${}^3F_3^o$		2.38(110)	3	3.275(99%)	3
		${}^1D_2^o$		1.480(89%)	1	6.54(136)	5
		${}^3D_1^o$		1.945(627)	4	8.663(87%)	5
		${}^3D_2^o$		2.003(650)	5	4.790(82%)	6
		${}^3D_3^o$		9.90(324)	5	6.260(99%)	5
		${}^3P_2^o$		5.36(102)	5	1.645(320)	7
		${}^3P_1^o$		2.775(522)	5	9.03(168)	6
		${}^1F_3^o$		8.15(134)	2	1.217(334)	5
		${}^1P_1^o$		1.096(256)	2	1.459(86%)	2
1D_2	$2p3s$	${}^3P_1^o$				6.732(99%)	2
		${}^3P_2^o$				7.629(99%)	2
		${}^1P_1^o$				8.306(99%)	4
	$2p3d$	${}^3F_2^o$		2.155(99%)	2	1.254(245)	7
		${}^3F_3^o$		5.437(99%)	1	4.72(266)	4
		${}^1D_2^o$		1.341(99%)	3	2.820(515)	7
		${}^3D_1^o$		3.316(99%)	1	1.898(99%)	3
		${}^3D_2^o$		5.890(99%)	2	7.90(191)	5
		${}^3D_3^o$		1.453(99%)	3	3.302(943)	3
		${}^3P_2^o$		3.511(99%)	2	4.44(110)	5
1S_0	$2p3s$	${}^3P_1^o$		5.739(99%)	2	1.223(99%)	3
		${}^1F_3^o$		3.116(76%)	5	4.790(539)	6
		${}^1P_1^o$		2.019(99%)	4	1.560(482)	6
	$2p3d$	${}^3D_1^o$				4.700(973)	4
		${}^3P_1^o$				7.217(95%)	5
		${}^3P_2^o$				3.69(108)	4
		${}^1P_1^o$				3.53(144)	2
		${}^1P_1^o$				1.205(669)	7

Table 6. (continued)

Multiplet		N II		O III		Si IX			
Lower	Upper	Present	x	Present	x	Present	x		
2p3s	$^3P_0^o$	2p ⁴	3P_1	2.787(421)	4				
		2p3p	1P_1	8.143(563)	3	3.720(130)	4		
			3D_1	2.795(227)	7	5.444(192)	7		
			3S_1	8.33(114)	6	1.676(132)	7		
			3P_1	3.148(171)	7	6.158(133)	7		
	$^3P_1^o$	2p ⁴	3P_0	8.29(123)	4				
			3P_1	2.010(292)	4				
			3P_2	1.903(274)	4				
			1D_2	6.546(99%)	1				
			1S_0	1.611(298)	4				
2p3p		1P_1	3.517(674)	6	3.771(150)	5	8.205(236)	7	
		3D_1	1.781(131)	7	3.846(137)	7	9.021(353)	7	
		3D_2	3.450(245)	7	7.360(260)	7	6.70(271)	8	
		3S_1	2.099(265)	7	4.618(364)	7	3.268(200)	8	
		3P_0	9.035(434)	7	1.961(42)	8	2.891(99%)	8	
		3P_1	2.120(109)	7	4.589(98)	7	1.089(19)	8	
		3P_2	2.224(106)	7	4.761(104)	7	3.13(124)	8	
		1D_2	1.205(240)	7	7.502(399)	4	4.49(188)	7	
	$^3P_1^o$	2p3p	1S_0	1.909(359)	7	1.469(57)	5	2.283(99%)	7
	$^3P_2^o$	2p ⁴	3P_1	3.128(436)	4				
2p3s			3P_2	5.281(709)	4				
			1D_2	1.744(99%)	3				
		1P_1	5.419(79%)	1	1.552(707)		1.650(603)	4	
		3D_1	1.262(101)	6	2.368(85)	6	5.224(73%)	6	
		3D_2	1.172(95)	7	2.222(79)	7	7.506(293)	7	
		3D_3	4.958(403)	7	9.609(341)	7	6.79(196)	8	
		3S_1	3.370(442)	7	6.326(500)	7	8.778(76%)	7	
		3P_1	4.388(256)	7	8.853(190)	7	3.34(230)	8	
		3P_2	7.482(420)	7	1.488(31)	8	6.960(110)	8	
		1D_2	7.783(507)	3	2.770(173)	4	3.624(154)	6	
2p3p	$^1P_1^o$	2p ⁴	3P_0	1.591(67)	1				
			3P_1	1.810(804)					
			3P_2	3.690(16)					
			1D_2	3.227(99%)	4				
			1S_0	1.375(354)	7				
		1P_1	2.583(176)	7	3.093(107)	7	1.119(40)	8	
		3D_1	2.386(442)	6	2.028(75)	5	4.526(149)	7	
		3D_2	3.273(654)	6	1.200(67)	4	5.37(221)	6	
		3S_1	2.434(473)	6	1.008(36)	5	2.873(71)	7	
		3P_0	8.53(161)	6	3.171(117)	4	2.094(99%)	6	
2p3p	1P_1	2s2p ³	$^1P_1^o$	2.306(452)	6	5.595(239)	4	4.424(90)	6
		2p3d	$^3F_2^o$	1.919(393)	6	1.282(191)	2	9.948(99%)	2
			$^1D_2^o$	1.216(75)	8	2.144(45)	8	2.139(866)	9
			1S_0	1.913(145)	8	3.577(264)	8	8.942(99%)	8
			$^3D_1^o$	1.761(171)	5	6.012(108)	5	7.730(275)	7
			$^3D_2^o$	6.32(175)	5	1.262(56)	5	4.204(55)	6

Table 6. (continued)

Multiplet			N II		O III		Si IX		
	Lower	Upper	Present	x	Present	x	Present	x	
2p3p	1P ₁	2p3d	³ P ₂ ^o	4.368(250)	4	9.796(308)	3	1.062(44)	6
			³ P ₁ ^o	1.647(218)	5	4.133(77)	5	1.325(76)	7
			³ P ₀ ^o	1.241(232)	2	4.411(541)	2	1.298(42)	6
			¹ P ₁ ^o	7.561(506)	7	1.844(31)	8	7.568(250)	8
			³ D ₁	3.257(99%)	2				
	2p3d		³ F ₂ ^o	9.644(266)	7	1.119(43)	8	1.456(22)	8
			¹ D ₂ ^o	1.866(162)	6	5.538(415)	7	3.136(109)	8
			³ D ₁ ^o	2.485(112)	7	4.796(9)	7	9.751(392)	7
			³ D ₂ ^o	3.066(269)	6	7.389(49)	6	1.682(88)	7
			³ P ₂ ^o	3.96(145)	4	6.70(157)	4	3.00(190)	4
3D ₂	2s2p ³		³ P ₁ ^o	1.589(565)	6	3.078(693)	6	3.871(797)	5
			³ P ₀ ^o	7.99(281)	6	1.703(379)	7	7.00(100)	7
			¹ P ₁ ^o	1.929(193)	5	7.468(138)	5	1.438(48)	8
			¹ P ₁ ^o	2.943(99%)	4				
			³ F ₂ ^o	1.587(53)	7	2.085(72)	7	4.934(99)	7
	2p3d		³ F ₃ ^o	1.036(28)	8	1.765(21)	8	4.692(100)	8
			¹ D ₂ ^o	2.174(99%)	3	6.864(592)	6	8.730(424)	6
			³ D ₁ ^o	7.733(341)	6	1.447(3)	7	2.633(129)	7
			³ D ₂ ^o	2.504(116)	7	4.746(15)	7	1.615(67)	8
			³ D ₃ ^o	1.919(184)	6	4.868(49)	6	1.222(56)	7
3D ₂	2p3d		³ P ₂ ^o	8.62(308)	5	1.574(359)	6	1.574(402)	6
			³ P ₁ ^o	6.44(228)	6	1.397(310)	7	6.501(900)	7
			¹ F ₃ ^o	5.210(494)	4	4.660(109)	4	1.802(117)	5
			¹ P ₁ ^o	6.77(161)	2	4.374(165)	2	2.018(294)	3
			³ F ₂ ^o	3.652(160)	5	4.628(192)	5	4.833(103)	5
	3D ₃		³ F ₃ ^o	1.044(39)	7	1.859(24)	7	3.250(75)	7
			³ F ₄ ^o	1.142(31)	8	1.948(23)	8	4.928(106)	8
			¹ D ₂ ^o	5.613(99%)	2	2.099(148)	5	7.044(203)	5
			³ D ₂ ^o	4.751(218)	6	8.585(29)	6	5.578(450)	6
			³ D ₃ ^o	3.167(148)	7	5.977(19)	7	2.036(84)	8
3S ₁	2p3d		³ P ₂ ^o	7.39(261)	6	1.608(358)	7	8.11(114)	7
			¹ F ₃ ^o	2.932(285)	3	7.547(390)	3	3.932(148)	5
			³ F ₂ ^o	4.82(101)	1	6.132(796)	2	1.722(99%)	
			¹ D ₂ ^o	3.107(286)	4	4.922(122)	3	2.053(589)	4
			³ D ₁ ^o	2.036(232)	5	7.068(136)	5	6.173(198)	7
	3P ₀		³ D ₂ ^o	3.689(380)	5	1.366(24)	6	1.661(30)	8
			³ P ₂ ^o	7.432(178)	7	1.457(24)	8	3.422(167)	8
			³ P ₁ ^o	7.112(157)	7	1.382(22)	8	2.784(114)	8
			³ P ₀ ^o	6.980(149)	7	1.351(22)	8	2.598(96)	8
			¹ P ₁ ^o	1.495(236)	5	3.453(85)	5	3.411(148)	7
3P ₁	3P ₀		³ D ₁ ^o	3.189(218)	7	5.949(68)	7	2.304(71)	8
			³ P ₁ ^o	9.83(107)	6	1.664(27)	7	1.637(83)	7
			¹ P ₁ ^o	3.877(817)	4	5.729(124)	4	1.162(57)	6
			³ F ₂ ^o	4.497(804)	4	4.862(358)	3	6.247(99%)	2
	3P ₁		¹ D ₂ ^o	2.566(683)	5	5.603(408)	4	4.069(57)	5
			³ D ₁ ^o	2.222(151)	7	4.030(48)	7	6.877(276)	7
			³ D ₂ ^o	4.227(295)	7	7.885(90)	7	1.877(65)	8
			³ P ₂ ^o	5.223(626)	6	7.435(132)	6	3.534(55)	7
			³ P ₁ ^o	1.113(129)	7	2.189(33)	7	2.322(59)	8

Table 6. (concluded.)

Multiplet			N II		O III		Si IX			
Lower	Upper		Present	x	Present	x	Present	x		
2p3p	3P_1	2p3d	$^3P_0^o$	3.700(412)	7	6.846(108)	7	3.858(110)	8	
			$^1P_1^o$	5.694(541)	3	2.920(47)	4	1.115(29)	6	
			$^3P_2^o$	1.709(301)	4	2.060(99)	4	2.249(67)	5	
			$^3F_3^o$	1.101(205)	5	6.341(433)	4	1.558(16)	5	
			$^1D_2^o$	5.873(92%)	3	2.416(594)	3	5.020(101)	5	
			$^3D_1^o$	1.291(91)	6	2.227(29)	6	1.294(99)	6	
			$^3D_2^o$	1.242(85)	7	2.190(27)	7	2.140(139)	7	
			$^3D_3^o$	5.468(373)	7	1.005(11)	8	3.194(104)	8	
			$^3P_2^o$	2.660(292)	7	4.862(74)	7	2.079(49)	8	
			$^3P_1^o$	1.439(157)	7	2.599(40)	7	9.570(255)	7	
			$^1F_3^o$	7.019(382)	3	1.687(135)	3	7.612(273)	5	
			$^1P_1^o$	3.34(100)	3	1.897(64)	3	8.05(504)	2	
1D_2			$^3F_2^o$	5.550(478)	4	2.834(241)	6	2.737(189)	6	
			$^3F_3^o$	1.010(102)	4	5.958(179)	3	6.844(624)	3	
			$^1D_2^o$	8.49(171)	6	7.79(110)	6	1.092(66)	7	
			$^3D_1^o$	1.906(296)	3	2.698(103)	3	3.484(219)	4	
			$^3D_2^o$	4.54(134)	4	5.513(414)	3	6.066(97)	5	
			$^3D_3^o$	6.606(430)	3	4.456(65)	3	3.67(101)	3	
			$^3P_2^o$	2.490(147)	4	3.971(66)	4	1.491(49)	6	
			$^3P_1^o$	1.433(383)	3	4.447(102)	2	1.894(98)	4	
			$^1F_3^o$	6.011(657)	7	1.277(29)	8	5.697(183)	8	
			$^1P_1^o$	4.63(191)	6	7.11(215)	6	1.840(428)	7	
1S_0			$^3D_1^o$	3.078(546)	3	4.132(73)	3	3.945(360)	4	
			$^3P_1^o$	1.036(221)	4	9.167(235)	3	3.318(327)	4	
			$^1P_1^o$	1.917(321)	7	3.325(185)	7	1.244(79)	8	
2p3d	$^3D_1^o$	$2p^4$	1S_0			4.16(113)	1			
			$^3P_1^o$			2.822(997)	1			
			$^1P_1^o$			1.830(821)	4			

Table 7. Comparison of experimental and theoretical transition rates (in 10^8 s^{-1}) for some transitions in N II.

Transition	$J - J'$	Musielok et al. [15]	Mar et al. [16]	CIV3 [13]	Present
$2p3s - 2p3p$	$^3P^o - ^3D$	2-3	0.484(44)	0.492	0.511
		1-2	0.328(30)	0.327	0.373
		0-1	0.268(21)	0.304	0.288
		2-2	0.114(10)	0.140	0.121
		1-1	0.178(16)	0.215	0.195
		2-1	0.0143(17)	0.018	0.0130
$2p3s - 2p3p$	$^3P^o - ^3S$	2-1	0.333(13)	0.369	0.332
		1-1	0.223(11)		0.219
		0-1	0.0874(48)		0.0822

for $2s2p^3$ $^3P_2^o - 2p3p$ 3D_1 in Si IX where the adjusted transition rates are $(1.0146, 1.0149) \times 10^8 \text{ s}^{-1}$ whereas our estimate is $1.02(68) \times 10^8 \text{ s}^{-1}$, most of the error arising from adjustment. At the same time, the discrepancy for intercombination lines is larger than we estimate, such as $(1.509, 1.980) \times 10^5 \text{ s}^{-1}$ for $2p^2$ 3P_2 – $2s.2p(3)$ $^5S_2^o$ in Si IX, whereas we estimate $1.509(50) \times 10^5 \text{ s}^{-1}$. This is an example where the velocity form of the Breit–Pauli line strength is in error.

Table 8. Comparison of some transition rates in O III (in s^{-1}) where Aggarawal [5] found considerable discrepancies. In the notation here, $+n$ implies that the preceding value is multiplied by 10^n .

Source	$2p^2 \ ^3P_2 - 2p3d \ ^3F_2$	$2p^2 \ ^3P_2 - 2p3d \ ^1F_3$	$2p^4 \ ^1D_2 - 2p3d \ ^1F_3$
CIV3 [5]	4.926+6	7.894+5	5.053+5
SS [18]	3.773+6	1.202+6	8.884+6
MCHF [17]	1.14+7	2.76+6	2.06+6
Present	9.165(197)+6	4.854(132)+6	3.11(76%)+5

Table 9. Comparison of several theoretical $2p3d \ ^3P_2$ decay rates in O III important in the Bowen fluorescence mechanism. Present values include uncertainty estimates in parentheses. The parameter x represents the factor 10^x that defines decay rates in s^{-1} .

Lower	Level	Present	MCHF [17]	SS [18]	x
$2p^2$	3P_1	2.091(35)	2.01	2.49	9
	3P_2	9.638(157)	9.40	12.9	9
	1D_2	1.022(25)	1.16	1.15	7
$2p^4$	3P_1	1.244(263)	3.47	3.99	5
	3D_1	6.710(1.57)	6.67	4.57	4
	3D_2	1.574(359)	1.57	1.50	6
	3D_3	1.608(358)	1.64	2.07	7
	3S_1	1.457(24)	1.42	1.50	8
	3P_1	7.435(132)	7.98	6.85	6
	3P_2	4.862(74)	5.21	4.20	7

6. Comparison with other theory and experiment

It is not possible here to include detailed comparisons with all similar data. Instead, we include some which we hope are a representative sample.

Table 7 compares our values with experimental measurements reported by Musielok et al. [15] and also by Mar et al. [16] as well as the CIV3 values. Agreement on the whole is excellent, though in slightly better agreement with the experimental data reported by Musielok et al. Our estimated uncertainties appear reasonable, although the last seems too large.

Aggarawal et al. [5] compare their results with some transition rates in O III from an earlier publication [17]. Generally agreement is good, but they mention three transitions where the discrepancy is especially large. In Table 8 we compare data for these three transitions including also the values obtained by Bhatia and Kastner [18]. The present results have changed slightly in the case of the $2p^2 \ ^3P_2 - 2p3d \ ^3F_2^o$, reducing by a factor of about two for $2p^2 \ ^3P_2 - 2p3d \ ^1F_3^o$, and increasing by almost an order of magnitude in the case of $2p^4 \ ^1D_2 - 2p3d \ ^1F_3^o$. It will be noticed, that the uncertainty in our present result for the latter is 76%. The large uncertainty arises largely from term energy corrections during the adjustment process. Aggarawal et al. attribute the discrepancy to the lack of correlation in the previous work [17] but that seems unlikely. What distinguishes these cases is the mixing of terms that need to be correctly predicted. $2p3d \ ^3F_2^o$ mixes strongly with $2p3d \ ^1D_2^o$, levels that are separated only by 271 cm^{-1} . In fact, the coefficient of the $2p3d \ ^3F^o$ component was 0.79 whereas the coefficient for $2p3d \ ^1D_2^o$ was 0.49 indicating extensive mixing of terms. On the other hand, $2p3d \ ^1F_3^o$ mixes with $2p3d \ ^3D_3^o$ where the levels are separated by 4469 cm^{-1} but the CIV3 calculations had a separation of 6847 cm^{-1} which could reduce a transition rate by more than a half. The mixing with $2p3d \ ^3D_3^o$ is not strong, but it should be noted that the $2p^2 \ ^3P_2 - 2p3d \ ^3D_3^o$ transition rate is particularly strong, and

Table 10. Comparison of intercombination transition rates (in s^{-1}) for $2p^2 \ ^3P_{J'} - 2s2p^3 \ ^5S_2^o$, and the lifetime (in ms) of the upper $^5S_2^o$ state in N II and O III. Uncertainties are given in units of the last digit quoted. The quantity Q is the decay rate to 3P_2 relative to 3P_1 .

$^3P_J - ^5S_2^o$		Q	Lifetime (ms)	Source			
1–2	2–2						
N II							
Theory							
50.83	124.79	2.455	5.69	Present (unadjusted)			
51.55	126.6	2.456	5.61(7)	Present (adjusted)			
		2.456	5.849	Froese Fischer 1999 [19]			
			6.4	Hibbert and Bates 1981 [23]			
			5.8	Dalgarno et al. 1981 [24]			
			3.2(1.6)	Cowan et al. 1982 [25]			
			6.45	Bell et al. 1995 [26]			
			5.43(3)	Hibbert 1996 [27]			
		2.44	5.43(0.3)	Brage et al. 1997 [28]			
Experiment							
			4.2(6)	Knight 1982 [29]			
			5.7(6)	Johnson et al. 1984 [30]			
			5.4(3)	Calamai and Johnson 1991 [31]			
			5.88(3)	Träbert et al. 2000 [32]			
O III							
Theory							
231.08	577.14	2.498	1.237	Present (unadjusted)			
230.8	576.5	2.498	1.239(18)	Present (adjusted)			
237	589	2.486	1.21(7)	Fleming and Brage 1997 [20]			
198.3	499.8	2.52	1.43	Froese Fischer and Saha 1985 [33]			
145	426	2.94	1.21(7)	Bhatia and Kastner 1993 [18]			
212	522	2.46	1.36	Nussbaumer and Storey 1981 [34]			
120	421	3.516	1.85	Cheng et al. 1979 [35]			
Experiment							
			1.22(8)	Johnson et al. 1984 [36]			
			2.91	Doschek and Feibelman 1993 [37]			
			1.22(8)	Träbert et al. 2000 [38]			

so a small mixing can have a large effect. Previous calculations did not include term energy corrections for transitions and accuracy then depends to a large extent on the accuracy of term energy separation.

The decay rates from the $2s^2 2p3d \ ^3P_2^o$ level are important in the study of the Bowen fluorescence mechanism. These too had been studied previously [17]. In Table 9, we compare our present results (including uncertainties) with earlier data and also data published by Bhatia and Kastner [18]. There is one significant difference from the earlier MCHF result, namely, the transition to $2p^4 \ ^3P_1$. The decay to $2s^2 2p3p \ ^3D_1$ has a large uncertainty but happens to be in good agreement with the earlier MCHF value. On the other hand, it is the transition with the smallest decay rate. All others are within 10% of the earlier Breit–Pauli calculations.

The $2s^2 2p^2 \ ^3P_J^o - 2s2p^3 \ ^5S_2^o$ line has been an intercombination line of considerable interest in astrophysical applications. In Table 10, we compare decay rates from $2s2p^3 \ ^5S_2^o$ to the two lower states $2s^2 2p^2 \ ^3P_{1,2}$ as well as the lifetime of the $^5S_2^o$ state. Theoretically, our present value of 5.61(7) ms *should* be more accurate (the model includes the effect of core-polarization of the $1s^2$ core) than the earlier work yielding a lifetime of 5.61(9) ms [19] for N II, not in quite as good agreement with the recent experimental value of 5.88 ± 0.03 ms as our earlier result. In O III, our results are in close agreement

Table 11. Lifetimes (in ns) for some levels in O III compared with experimental values and other theories. Previous results are from ref. 17 and Wiese et al. from ref. 21.

Level	Term	Present	Previous	Wiese et al.	Experiment	Source
$2s2p^3$	$^3S^o$	0.0699(57)	0.078	0.07(4)	0.0960(124) 0.105(12) 0.079(4)	Lin et al. [39] Heroux [40] Pinnington et al. [41]
	$^3P^o$	0.544(8)	0.534		0.575(18)	Pinnington et al. [41]
	$^3D^o$	1.629(18)	1.59		1.61(7)	Pinnington et al. [41]
	$^1D^o$	0.183(2)	0.18	0.15(7)	0.13(2) 0.20(5)	Lin et al. [39] Pinnington et al. [41]
$2p^4$	3P	0.165(14)	1.55		0.166, 0.18, 0.176	Pinnington et al. [41]
$2p3s$	$^3P^o$	0.254(42)	0.266	0.26(13)	0.34(5)	Lin et al. [39]
$2p3s$	$^1P^o$	0.212(41)			0.17(1)	Baudinet-Robinet et al. [42]
$2p3p$	$^3D^o$	5.326(96)	4.4		11(1) 7.6, 8.6 8.9(2)	Martinson et al. [43] Church and Liu [44] Pinnington et al. [41]
	$^3S^o$	2.373(94)	1.92		2.8(1) 2.9(2) 3.13(14)	Cardon et al. [45] Berry et al. [46] Pinnington et al. [41]
	$^3P^o$	2.949(112)	3.2		2.5(4)	Pinnington [47]

with those of Fleming and Brage [20]. The lifetime is in good agreement with the two experiments that are exactly the same.

Table 11 compares the lifetimes of a number of levels with our earlier predictions [17] and various experiments. When several of the latter are quoted, they are in chronological order. Generally, the present results are in better agreement with the latest experiment, but agreement is far from perfect, particularly for lifetimes of $2p3p$ states.

7. Conclusions

In this paper we have presented lifetime data for a portion of a spectrum in the carbonlike isoelectronic sequence. Results are based on simultaneous optimization of orbitals for a number of terms and the diagonalization of the Breit–Pauli Hamiltonian (omitting orbit–orbit). Data for N II, O III, and Si IX have been further refined through the inclusion of term energy corrections. These results, together with discrepancies in transition energy and line strengths, have allowed us to determine an uncertainty estimate. The latter includes the change in the transition rate through the normalization and hence, can also be considered an indicator of reliability for the unadjusted data included at the Web site.

The large Breit–Pauli calculations were performed on the T3E at the National Energy Research Scientific Computing Center (NERSC) using an MPI version of the code and employing 64 processors for the larger cases.

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